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**MODELING PHASE CHANGE MATERIAL IN MICRO-
FOAM UNDER CONSTANT TEMPERATURE CONDITION
(POSTPRINT)**

Soumya S. Patnaik

**Mechanical and Thermal Systems Branch
Power and Control Division**

Xin Hui

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*//Signature//

SOUMYA S. PATNAIK
Program Manager
Mechanical and Thermal Systems Branch
Power and Control Division

//Signature//

THOMAS L. REITZ, Technical Advisor
Mechanical and Thermal Systems Branch
Power and Control Division
Aerospace Systems Directorate

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Modeling phase change material in micro-foam under constant temperature condition



Xin Hu^{a,b}, Soumya S. Patnaik^{b,*}

^a UES, Inc., 4401 Dayton-Xenia Road, Dayton, OH 45432-1894, USA

^b Aerospace Systems Directorate, Air Force Research Laboratory, Dayton, OH 45433-7251, USA

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ABSTRACT

Heat transfer of phase change material (PCM) in an open cell micro-foam structure was numerically studied. A high constant temperature was specified at the top surface of the structure. Each unit of the micro-foam is a body-centered-cubic (BCC) lattice embedded with spherical micro-pores. Two different simulation methodologies were applied. One is the high-fidelity direct numerical simulation (DNS), which allows for the effective thermo-physical parameters to be derived. The other methodology is a volume-averaged simulation based on one- and two-temperature models. Our results show that the volume-averaged simulation can accurately and efficiently capture the phase change process in PCM/micro-foam systems, with the effective thermal conductivity derived from direct simulations and expressed as a power law of porosity.

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1. Introduction

Metal or graphite foams [1] filled with phase change materials (PCM) are attractive for thermal energy storage (TES) [2] particularly in high heat flux applications as they provide both high storage capacity and short time constants. The latent heat of PCM provides high heat capacity whereas the foam structure increases the effective thermal conductivity. In earlier studies of phase change materials in foams, the volume-averaged (macroscopic) approach such as one-temperature and two-temperature models has been used, in which either local thermal equilibrium (LTE) between PCM and foams was assumed, or the simplified Newton's cooling law was applied [3,4]. The volume-averaged simulation can be effective for porous structure with simple geometry, however, this method can be restrictive for the modeling of foams with complex geometry. The complex foam structure which affects the effective thermal conductivity and interstitial heat transfer coefficient and subsequently the PCM melting/solidification needs to be accurately modeled to provide a better understanding of the heat transfer behavior of the system. The conventional method of effective thermal conductivity derived from packed bed with discrete solid particles as is done for simple porous structures cannot be

applied here without modification and more accurate methods such as direct numerical simulation are required.

In this paper, we investigate the phase change in a low porosity micro-foam using both volume-averaged and direct numerical simulation [5]. The foam was modeled as an ideal structure with BCC unit lattice and spherical micro-pores. The temperature at the top surface of the porous structure was kept constant. The objective of this work is to compare various simulation methodologies and identify one that can model the heat transfer process in PCM and micro-foam structure with sufficient efficiency and accuracy. The volume-averaged simulations were carried out using one- and two-temperature models, whereas in the DNS, separate energy equations were applied to micro-foam and PCM domains and conjugate heat transfer was considered on the interface. Results including melted PCM volume fraction, temperature difference between PCM and micro-foam, instantaneous temperature profile, and heat flux are discussed.

2. Model and methods

2.1. Physical model

The physical model and geometry of the simulated micro-foam is shown in Fig. 1. A cube with the side length of 2.56 cm was used for volume-averaged simulations (Fig. 1a). The top surface was held at several constant temperatures ($T_{top} = 334, 351, \text{ or } 368 \text{ K}$), and the other surfaces were insulated. In direct numerical simulation (Fig. 1b), the micro-foam geometry was composed of a series

* Corresponding author. Address: Thermal and Mechanical Branch, Air Force Research Laboratory, 1950 Fifth Street, Bldg 18, WPAFB, OH 45433, USA. Tel.: +1 9376565452; fax: +1 9376564132.

E-mail addresses: xin.hu.ctr@wpafb.af.mil (X. Hu), soumya.patnaik.1@us.af.mil (S.S. Patnaik).

Nomenclature

Alphabetic symbols

A_{fs}	area of PCM/micro-foam interface
c_p	specific heat
H	side length of cube
h_{fs}	interstitial heat transfer coefficient
h_v	volumetric heat transfer coefficient
k	thermal conductivity
L	latent heat of fusion
r_d	distance from the cell centroid to the top surface
s	ratio of PCM surface area to the total area on the top boundary
T	temperature
T_m	melting temperature of PCM
t	time

q'' heat flux

Greek symbols

α	power factor in Progelhoff model
ρ	density
γ	porosity (0–1)
δT	temperature difference between micro-foam and PCM

Subscripts

eff	effective value
ini	initial condition
Top	top surface of the simulation domain
s	solid (micro-foam)
f	fluid (melted PCM)

of unit cells, and each was represented by a solid cube (side length of 400 μm) with nine spherical pores arranged in a BCC lattice [5–7]. The length in Y-direction was kept the same as that in the volume-averaged simulations and comprises of 64 unit cells. The X & Z lengths are much smaller (0.02 cm) to keep the mesh size and computation time at an affordable level. The top surface of the unit-cell array is specified with the same temperature condition as that in the volume-averaged simulations. The bottom surface of the unit-cell array was insulated. Symmetric conditions were specified at other surfaces. The initial temperature of PCM/micro-foam system was 300 K in both volume-averaged and direct simulations.

We considered aluminum foam and docosane (paraffin wax with $\text{C}_{22}\text{H}_{46}$ composition) PCM whose melting temperature of 317 K is below the top-wall temperature. It was assumed that the micro-foam is fully saturated with docosane and there is no volume change of PCM. All thermo-physical parameters of these two materials (Table 1) were kept constant in the simulations.

The foam porosity was 0.757 and pore size is 360 μm for the current simulations. The fluid flow within the melted PCM region can be neglected because such low porosity micro-foam provide a dominant resistance force to suppress the flow driven by the natural convection [8]. Thus, only the energy equations were solved in the simulations.

2.2. Direct numerical simulation of PCM in foam

Without the need for extra ad hoc assumptions such as local thermal equilibrium (LTE), direct numerical simulations are considered as much closer to the real situation. In DNS, various energy equations were applied to PCM and the foam domains respectively, as shown in the following:

Table 1
Thermo-physical parameters for PCM and micro-foam.

	ρ (kg/m ³)	c_p (kJ/kg-K)	k (W/m-K)	L (kJ/kg)	T_m (K)
PCM	785	2.89	0.4	260	317
Micro-foam	2719	8.71	202.4	N/A	N/A

$$\rho_f c_{pf} \frac{\partial T_f}{\partial t} = \nabla \cdot (k_f \nabla T_f) - \rho_f L \frac{\partial f_l}{\partial t} \quad (1)$$

$$\rho_s c_{ps} \frac{\partial T_s}{\partial t} = \nabla \cdot (k_s \nabla T_s) \quad (2)$$

Conjugate heat transfer was considered at the PCM/micro-foam interface:

$$\left. \begin{aligned} T_f &= T_s \\ k_f \frac{\partial T_f}{\partial n} &= k_s \frac{\partial T_s}{\partial n} \end{aligned} \right\} \quad (3)$$

Subscripts f and s in Eqs. (1)–(3) stand for PCM and foam respectively; ρ , c_p , T , t , k , and L are density, specific heat, temperature, time, thermal conductivity and latent heat of fusion. In the right hand side of Eq. (1), f_l is the volume fraction with the value of 1 in the melted PCM region, 0 in the solid PCM region, and 0–1 in the mushy region. Effects of porosity and pore size have been directly included in the ideal foam geometry.

2.3. One-temperature simulation of phase change in foam

One-temperature model assumes that PCM and the micro-foam have the same temperature. Therefore only one energy equation is applied for the whole system:

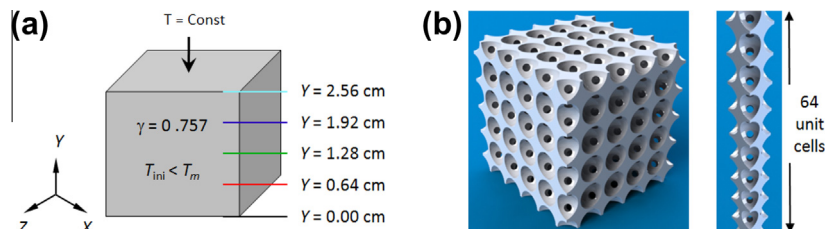


Fig. 1. (a) Geometry and thermal boundary conditions in volume-averaged simulation; (b) ideal foam microstructure (PCM not shown) in direct simulation. The top surface is held at a constant temperature.

$$(\gamma \rho_f c_{p,f} + (1 - \gamma) \rho_s c_{p,s}) \frac{\partial T}{\partial t} = \nabla \cdot (k_{eff} \nabla T) - \rho_f \gamma L \frac{\partial f_l}{\partial t} \quad (4)$$

where γ is the porosity, with value 1 standing for pure solid. The effective thermal conductivity k_{eff} is a function of porosity, thermal conductivity of each component, and more importantly, the detail structure of the foam. The simplest and commonly used expression $k_{eff} = \gamma k_f + (1 - \gamma) k_s$ is essentially the arithmetic mean. In PCM/micro-foam system, a more accurate k_{eff} can be obtained by experiments [9–11], or by DNS of real or ideal foam geometries [5–7,12–14]. In this paper, we have carried out DNS to find the effective thermal conductivity, which matches the Progelhoff model [15] $k_{eff} = \gamma k_f + (1 - \gamma)^\alpha k_s$ with $\alpha = 1.31$ through curve fitting, when pores in ideal foam structure is arranged in a BCC lattice [16].

2.4. Two-temperature simulation of phase change in foam

In two-temperature model, energy equations for PCM and foam need to be considered separately because of the local thermal non-equilibrium (LTNE). Their heat transfer is modeled by the Newton's law of cooling:

$$\gamma \rho_f c_{p,f} \frac{\partial T_f}{\partial t} = \nabla \cdot (k_{f,eff} \nabla T_f) - \rho_f \gamma L \frac{\partial f_l}{\partial t} - h_v (T_f - T_s) \quad (5)$$

$$(1 - \gamma) \rho_s c_{p,s} \frac{\partial T_s}{\partial t} = \nabla \cdot (k_{s,eff} \nabla T_s) - h_v (T_s - T_f) \quad (6)$$

where effective thermal conductivities for PCM $k_{f,eff}$ and for the foam $k_{s,eff}$ are still related to foam structure. Here we used two sets of effective thermal conductivities: one corresponds to the arithmetic mean such that $k_{f,eff} = \gamma k_f$ and $k_{s,eff} = (1 - \gamma) k_s$. The other corresponds to the Progelhoff model, with $k_{f,eff} = \gamma k_f$ and $k_{s,eff} = (1 - \gamma)^\alpha k_s$ respectively. The volumetric heat transfer coefficient $h_v = A_{fs} h_{fs}$, where the specific surface area A_{fs} is the ratio of interstitial surface area to the representative elementary volume (REV), and h_{fs} is the interstitial heat transfer coefficient between PCM and foam. Both h_{fs} and A_{fs} are highly dependent on the foam structure. In this work, the specific surface area $A_{fs} = 1.08 \times 10^4 \text{ m}^{-1}$ is obtained from the foam structure described in Section 2.1. The interstitial heat transfer coefficient is defined as $h_{fs} = q''_{fs} / (\bar{T}_s - \bar{T}_f)$, where q''_{fs} is the heat flux at the fluid/foam interface, \bar{T}_s is the volume-weighted average temperature for micro-foam and \bar{T}_f is the mass-weighted average temperature for fluid. The interstitial heat transfer coefficient h_{fs} is calculated in a similar manner as that by Krishnan et al. [6,7]. We applied direct simulation on the unit-cell level, and based on the calculated heat flux across the interface and the average PCM and foam temperatures we obtained the value of interstitial heat transfer coefficient $h_{fs} = 9.09 \times 10^3 \text{ W}/(\text{m}^2 \text{ K})$.

2.5. Problem setup

For these simulations, the commercial CFD package ANSYS FLUENT 13.0 was used with double precision. Parallel and batch processing were carried in the AFRL DoD Supercomputer Resource Center (DSRC). To apply the two-temperature model in FLUENT, a user-defined scalar (UDS) was used for micro-foam temperature. The convergence criterion of absolute scaled residual for energy equation was set to be 10^{-9} for volume-averaged simulations and 10^{-11} for DNS. Grid- and time-step-independent results were ensured first. We found that the grid with 90 k cells and time step size $dt = 0.02 \text{ s}$ are enough for one- and two-temperature simulations, while we used the grid with 9 million cells and $dt = 0.008 \text{ s}$ for direct simulations. A typical DNS needed over 30,000 CPU hours (i.e., 192 CPU cores for around 160 h), much more expensive than volume-averaged simulations.

3. Results and discussion

The direct numerical simulations show very complicated micro-scale evolutions of melting front and temperature distributions, which are very different from the one-dimensional macro-scale behavior distributions generated by the volume-averaged simulations. In order to compare different simulation techniques, we studied heat transfer behavior such as the volume fraction of melted PCM, average temperature at different locations, temperature difference between micro-foam and PCM, and the top-wall heat fluxes.

3.1. Volume fraction of melted PCM

Fig. 2 shows the profiles of melted PCM volume fraction with top surface temperature fixed at 334 K and 368 K respectively. Here “1-T” and “2-T” stand for one- and two-temperature simulations. “Arithmetic Mean” and “Progelhoff” refer to the arithmetic mean and Progelhoff models for the effective thermal conductivity. First, we can see that one- and two-temperature simulations with the arithmetic mean predict higher melting rate than those from Progelhoff model and the DNS. This is because the arithmetic mean generates higher effective thermal conductivity, thus enables system absorbing more heat to melt PCM quickly. Second,

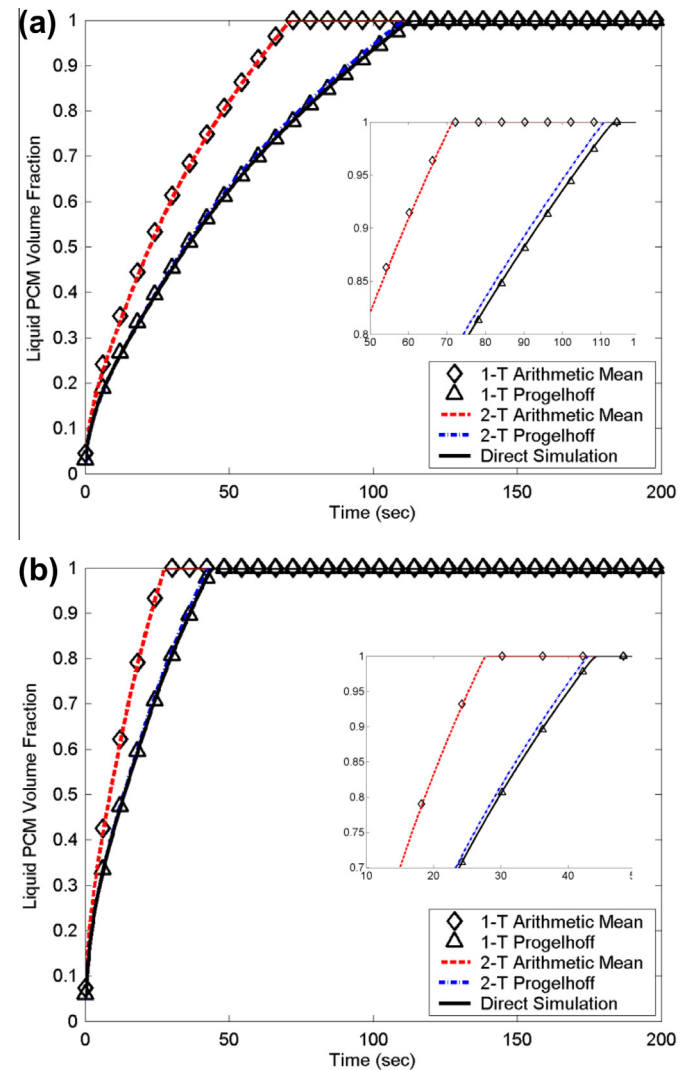


Fig. 2. Profiles of melted PCM volume fraction: (a) $T_{top} = 334 \text{ K}$; (b) $T_{top} = 368 \text{ K}$.

one-temperature and two-temperature simulations accurately predict volume fraction of melted PCM, when the Progelhoff model is used for the effective thermal conductivity k_{eff} . Hence, modeling of k_{eff} plays a key role in the volume-averaged simulation. As prescribed by Progelhoff model, k_{eff} nonlinearly depends on the porosity, and is dominated by the thermal conductivity of micro-foam. As the enforced top surface temperature is raised (Fig. 2b), the temperature gradient at the top surface increases and induces an earlier melting of PCM.

3.2. Average temperature at different Y-cross sections

Fig. 3 shows the time history of area-weighted average temperature at two cross sections in the foam, with the top-surface temperature fixed at 334 K. At a cross section close to the top surface (Fig. 3a), the temperature simulated from volume-averaged method and Progelhoff model reasonably fit the results from DNS. Arithmetic model of effective thermal conductivity, however, seemingly over-estimates the temperature change by 12% in the phase change region compared to DNS.

At the bottom of the system (Fig. 3b) this over-estimation gets worse. When the effective thermal conductivity is calculated from arithmetic mean, the volume-averaged simulation predicts earlier starting time of phase change compared to direct simulation

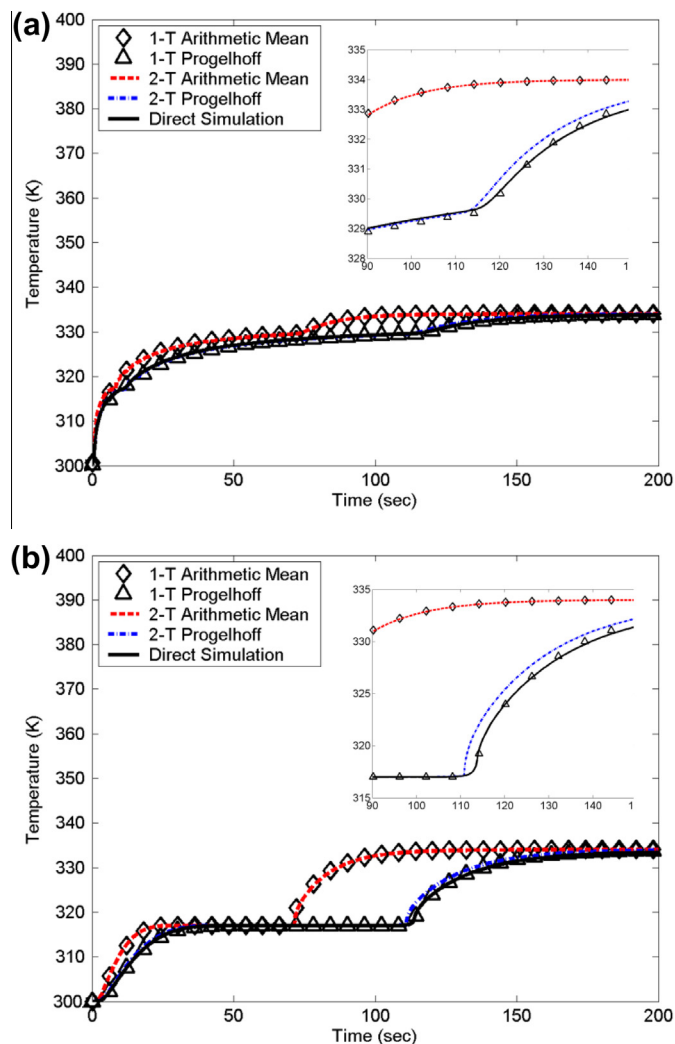


Fig. 3. Average temperature profiles at (a) cross section $Y = 1.92$ cm, and (b) bottom plane $Y = 0.0$ cm. The top-surface temperature $T_{top} = 334$ K.

(Fig. 3b), indicating the over-estimation of the effective thermal conductivity of PCM/foam system by arithmetic mean. When the Progelhoff model is applied to calculate k_{eff} , the temperature variation is well captured, no matter whether one-temperature or two-temperature simulation is conducted. It is noteworthy that there is a temperature plateau at the structure bottom (Fig. 3b), in which heat transfer is primarily dominated by phase change. In contrast, the average temperature at the cross section near the top surface (Fig. 3a), indicating the fast rising temperature of foam structure at this cross section due to its high conductivity. As the cross section moves toward the bottom, the heat conduction through foam structure slows down, and the phase change process is more pronounced.

3.3. Temperature difference between micro-foam and PCM

In two-temperature and direct numerical simulations, the effective thermal conductivity and the interstitial heat transfer are two competing factors affecting the thermal process between micro-foam and PCM. Larger differences in values of effective thermal conductivities between micro-foam and PCM induces larger temperature difference between them; while a stronger interstitial heat transfer makes the temperature jump smaller. Comparison of temperature difference cross the micro-foam and PCM interface $\delta T = T_s - T_f$ will help us better evaluate the two-temperature simulation.

The temperature differences at two cross sections ($Y = 1.92$ cm and 0.0 cm) from two-temperature and direct simulations are shown in Fig. 4. The onset of phase change (melting) is indicated by the peak, which separates pre- and post-melting stages. With results from direct simulations as the reference, we can see that the two-temperature simulation using arithmetic mean model predicts earlier melting stages in both Y-locations, and the peak magnitude is dramatically over-estimated at the cross section close to the top surface ($Y = 1.92$ cm). However, two-temperature simulations using Progelhoff model predicts acceptable time onset of melting process and the temperature difference. With the cross section further away from the top-wall (e.g., at $Y = 0.0$ cm), the discrepancy in the melting onset is more obvious.

Temperature difference under a higher top-wall temperature ($T_{top} = 368$ K) is presented in Fig. 5. The melting onset is advanced as the top-wall temperature is increased. We can see that

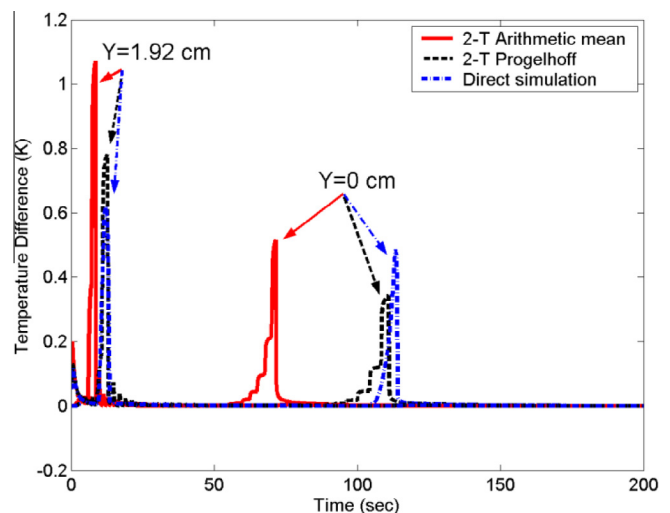


Fig. 4. Comparison of temperature difference between micro-foam and PCM ($T_{top} = 334$ K).

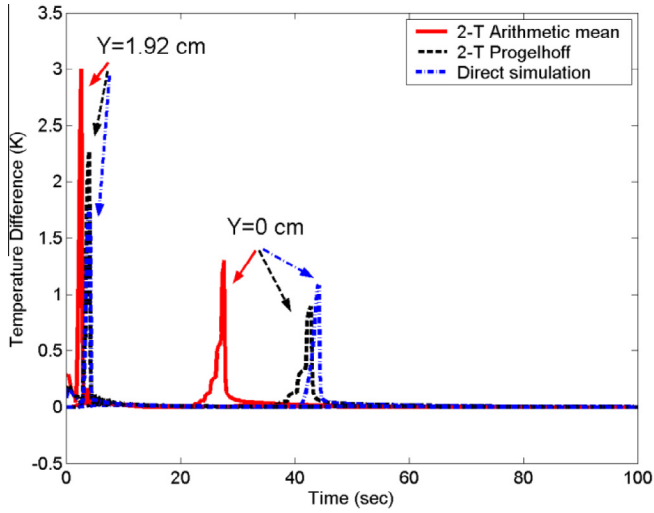


Fig. 5. Comparison of temperature difference between micro-foam and PCM ($T_{top} = 368$ K).

two-temperature simulation with Progelhoff model predicts nearly the same starting time of phase change as that from direct simulation in both cross sections.

3.4. Heat flux at top surface

We further calculated the area-weighted average heat flux at top surface using various simulation methodologies. In one-temperature simulation, only the overall top-wall heat flux can be calculated. In two-temperature simulation and DNS, we can calculate the top-wall heat flux for each component, i.e., the amount of heat flows through the PCM and through micro-foam respectively. The overall heat flux at the top surface is just the sum of heat flux from PCM and the foam, i.e., $q''_{top} = sq''_{f,top} + (1-s)q''_{s,top}$, where s is the area ratio of PCM surface area to the total on the top surface. The heat flux of the foam is defined as $q''_{s,top} = \frac{k_{eff,s}(T_{s,cell@top} - T_{top})}{r_d}$, in which $T_{s,cell@top}$ is the foam temperature at the centroid of a cell near the top surface, and r_d is the distance from the cell centroid to the top surface. In the current study, both the overall and individual heat fluxes at the top surface are normalized by the upper limit heat flux, which is defined as $q''_{max} = H\{\gamma\rho_f L + (\gamma\rho_f c_{p,f} + (1-\gamma)\rho_s c_{p,s})(T_{top} - T_{ini})\}$. H is the distance from the top to the bottom surface, and is the cube length in our case.

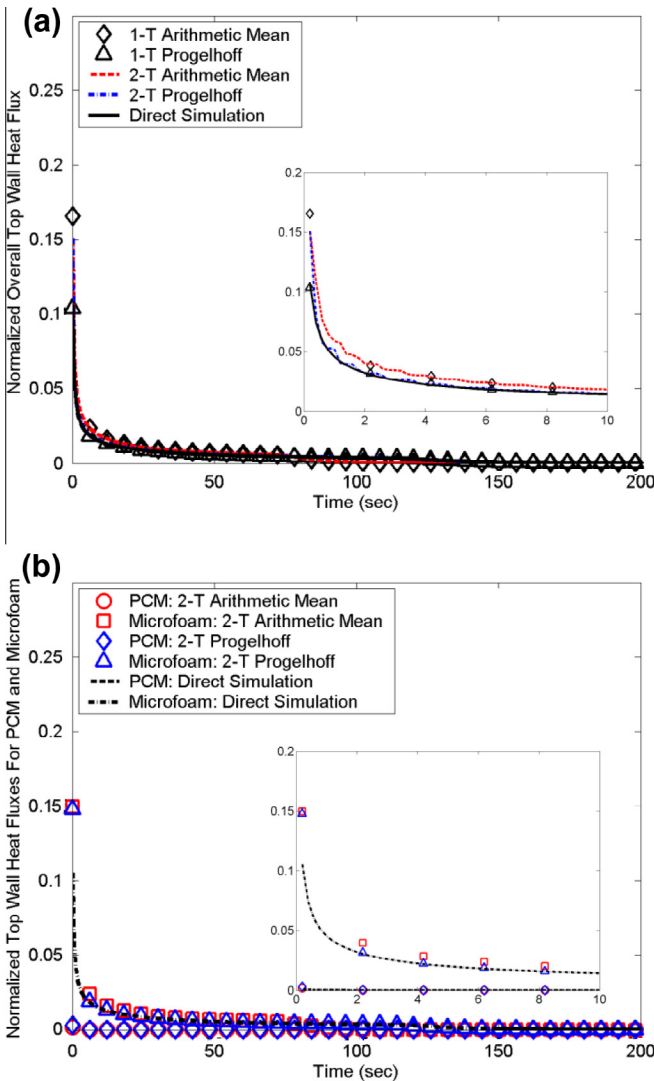


Fig. 6. Heat flux at top surface (a) overall (b) individual component ($T_{top} = 334$ K).

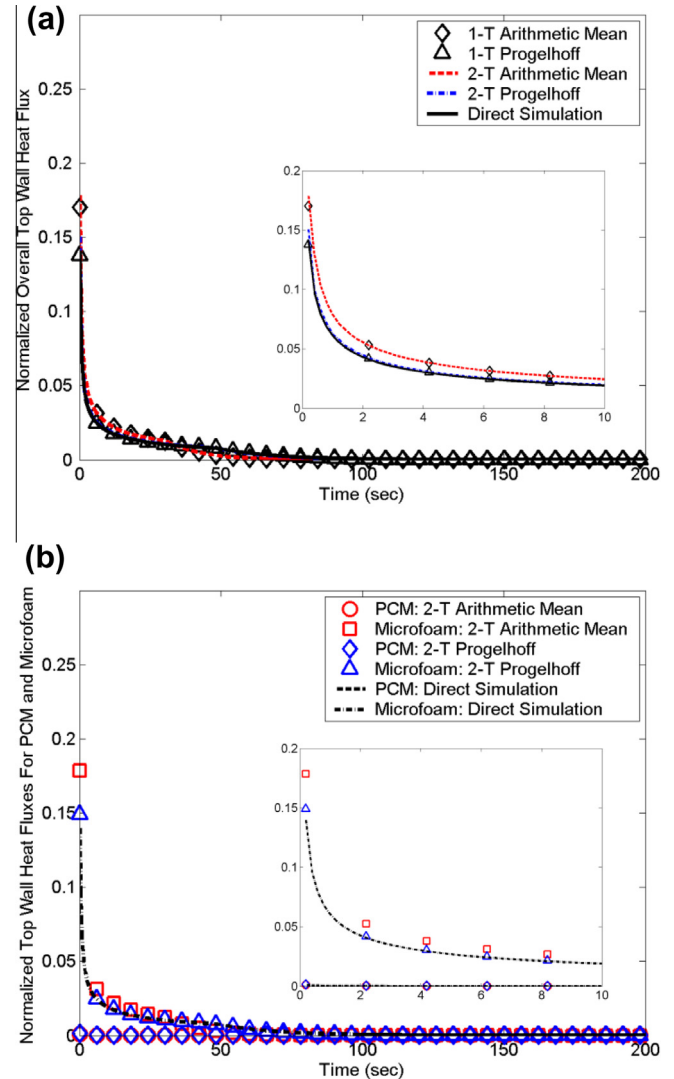


Fig. 7. Heat flux at top surface (a) overall (b) individual component ($T_{top} = 368$ K).

Fig. 6(a) shows the normalized overall heat flux at top surface. Volume-averaged simulations predict the heat flux reasonably well. However, the effective thermal conductivity calculated from Progellhoff model generates more accurate results than from arithmetic mean model (Fig. 6(a) insert). The heat flux of individual material components is presented in Fig. 6(b). From the insert, it can be seen that the heat flux from the micro-foam is much larger than that from PCM, since the thermal conductivity of the micro-foam is three orders of magnitude higher than that of PCM. (Table 1).

We also calculated the overall and individual heat fluxes on the top surface, at which the temperature T_{top} is raised to 368 K (Fig. 7). The flux is increased at the top surface, contributed principally by the micro-foam. It is worth mentioning that, unlike the temperature at various cross sections, the heat flux gradually and slowly approaches a steady value. This can be ascribed to the varying effective thermal conductivity and temperature gradient in the system.

4. Conclusions

In this work, we numerically studied the heat transfer behavior of a phase change material in an open-cell micro-foam using both volume-averaged and direct simulations. Heat transfer process was simulated for a spherical-pore embedded micro-foam, and its top surface was kept isothermal. By examining the volume fraction of melted PCM, average temperature at different locations, temperature jump across micro-foam and PCM interface, and average heat flux at the top surface, we find that volume-averaged simulations can reasonably predict the heat transfer process in the micro-foam with complex geometry, as long as accurate thermo-physical parameters such as effective thermal conductivity are provided. In the present study, the effective thermal conductivity of the PCM/micro-foam system was obtained from direct numerical simulation of a unit cell. The simulations results supported the Progellhoff model of effective thermal conductivity where the effective thermal conductivity can be expressed as a power law of porosity and a power factor of 1.3 was calculated for the model structure. We found that the heat flux near the enforced isothermal boundary is dominated by the micro-foam due to its high thermal conductivity. The phase change heat transfer becomes gradually more pronounced in locations away from the enforced high temperature boundary.

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